Mathematical model suitable for simulations of thin semi-flexible polymers

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We present an alternative approach [1] to simulations of semi-flexible polymers. In contrast with the usual bead-rod compromise between bead-spring and rigid rod models, we use deformable cylindrical segments as basic units of the polymer. The length of each segment is not preserved with end points diffusing under constraints keeping the polymer chain nature intact. The model allows the simulation of tension transport and elasticity properties. In particular we describe a new cooperative regime in the relaxation of the polymer from its fully elongated configuration.

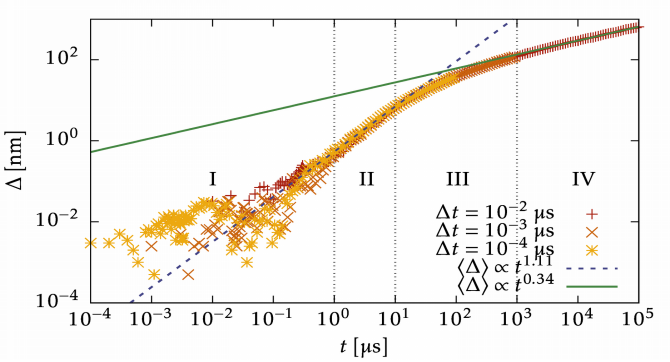

Figure 1: *Log-log plot of the time dependency of thepolymer's end point displacement during the relaxationof the polymer from straight configuration. The newcooperative regime is denoted as II.*

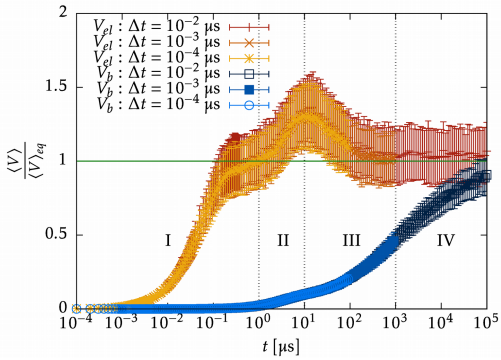

Figure 2: *Semi-log plot of the bending and elasticenergy during the relaxation of the polymer.*

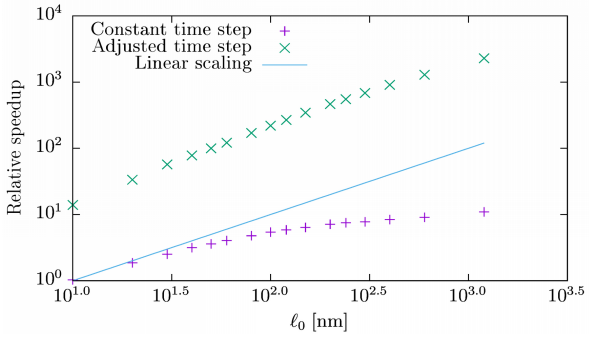

Figure 3: *The dependency of the speed-up of our model relative to the bead-spring model on the segment length.*

References

[1] Pešek, J., Baerts, P., Smeets, B., Maes, C. and Ramon, H., Soft matter, 12, 3360-3387 (2016)